

# Bell-CHSH function approach to quantum phase transitions in matrix product systems

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**Abstract.** Recently, nonlocality and Bell inequalities have been used to investigate quantum phase transitions (QPTs) in low-dimensional quantum systems. Nonlocality can be detected by the Bell-CHSH function (BCF). In this work, we extend the study of BCF to the QPTs in matrix product systems (MPSs). In this kind of QPTs, the ground-state energy keeps analytical in the vicinity of the QPT points, and is usually called the MPS-QPTs. For several typical models, our results show that BCF can signal the MPS-QPTs very well. In addition, we find BCF can capture signal of QPTs in unentangled states and classical states, for which other measures of quantum correlation (quantum entanglement and quantum discord) fail. Furthermore, we find that in these MPSs, there exists some kind of quantum correlation which cannot be characterized by entanglement, or by nonlocality.

Submitted to: *J. Phys.: Condens. Matter*

## 1. Introduction

Quantum phase transition (QPT) is a very interesting phenomenon in many-body quantum systems.[1] Compared with the classical phase transitions driven by thermodynamic fluctuation, QPTs occur at zero temperature, thus the thermodynamic fluctuation is absent. In fact, QPTs are driven by the so-called quantum fluctuation. For a quantum system described by a Hamiltonian  $\hat{H}(g)$  with  $g$  the tuning parameter, the ground-state property (i.e. the ground-state energy) of  $\hat{H}(g)$  may show qualitative change at some point  $g_c$ , then a QPT occurs. Most QPTs, such as various magnetization transitions in spin models,[1, 2] can be investigated by traditional order parameters. It needs mention that, some exotic QPTs, such as the topological QPT,[3] cannot be described by local order parameters.

In the vicinity of the QPT point, long-range correlations would develop in the ground state. Thus it is expected that quantum correlation plays a central role in the QPTs.[7, 3, 5, 1, 4, 6, 2] Quantum entanglement is the most famous measure of quantum correlation. For various models, it has been found that the entanglement is singular in the vicinity of the QPT points, which is usually related to the singularity of the ground-state energy at the QPTs.[2, 8] Nonlocality is another aspect of quantum correlation, and can be indicated by the violation of Bell inequalities, such as the famous Bell-Clauser-Horne-Shimony-Holt (CHSH) inequality.[10, 5, 6, 11, 12, 9, 13] For a long time, nonlocality and entanglement were regarded as identical. In fact, for pure two-qubit states, it has been proved rigorously by Gisin that the two are indeed equivalent.[14] However, for mixed states, it's found that an entangled state may not violate any Bell inequality, i.e., an entangled state is not necessarily a non-local state.[15] Thus, nonlocality and entanglement turn out to be two different aspects of quantum correlation.

Quite recently, it has been found that the Bell-CHSH function (BCF), which is associated with the Bell-CHSH inequality, can serve as a useful QPT detector, even for topological QPT[3, 16] and Kosterlitz-Thouless QPT[5]. It should point out that a complete understanding about the features of BCF in detecting QPTs has not yet been reached.

In this work, we make a further step by considering an exotic type of QPTs occurring in the so-called matrix product states(MPSs).[23, 17, 21, 22, 18, 19, 20] In this kind of QPTs, the ground-state energy remains analytic in the entire parameter space, thus the situation is different from traditional QPTs.[19] In order to distinguish them from traditional QPTs, we usually call them MPS-QPTs. The MPSs have always provided a valuable test-bed for understanding the features of various QPT detectors, including quantum entanglement,[17, 22] quantum discord[23] and quantum fidelity[21, 22]. In this work, we investigate the ability of BCF to detect QPTs by considering MPS models. Firstly, as we will show, several typical MPSs display clearly the features of BCF in detecting QPTs. Secondly, MPSs help us understand the role of quantum correlation, quantum entanglement, and nonlocality in QPTs.

## 2. Bell-CHSH inequality, entanglement concurrence, and quantum discord

Bell-CHSH inequality is the simplest nontrivial Bell inequality. First, let's define the CHSH operator as  $\hat{B} = \hat{A}_1 \otimes \hat{B}_1 + \hat{A}_1 \otimes \hat{B}_2 + \hat{A}_2 \otimes \hat{B}_1 - \hat{A}_2 \otimes \hat{B}_2$ , where  $\hat{A}_i = \vec{a}_i \cdot \vec{\sigma}$  and  $\hat{B}_i = \vec{b}_i \cdot \vec{\sigma}$ , with  $\vec{a}_i$  and  $\vec{b}_i$  unit vectors and  $\vec{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ . Then for any realistic and local two-qubit state  $\hat{\rho}_2$ , the Bell-CHSH inequality reads  $|\langle \hat{B} \rangle| = |\text{Tr}(\hat{\rho}_2 \hat{B})| \leq 2$ .  $|\langle \hat{B} \rangle|$  depends upon the vectors  $\vec{a}_i$  and  $\vec{b}_i$ , and one can optimize  $|\langle \hat{B} \rangle|$  over all vectors  $\vec{a}_i$  and  $\vec{b}_i$  to get the maximum value  $B(\hat{\rho}_2) = \max_{\{\vec{a}_i, \vec{b}_i\}} |\langle \hat{B} \rangle|$ . [12, 10, 9] We will refer to  $B(\hat{\rho}_2)$  as the Bell-CHSH function (BCF) in this work. For some state  $\hat{\rho}_2$ , if it turns out that  $B(\hat{\rho}_2) > 2$ , we usually say that the Bell-CHSH inequality is violated, which means that the state  $\hat{\rho}_2$  cannot be described by a realistic local theory, in other words, it is non-local.

Alternatively, it's found by Horodeckis that for any two-qubit state

$$\hat{\rho}_2 = \begin{pmatrix} x_{11} & o_{12} & o_{13} & x_{14} \\ o_{21} & x_{22} & x_{23} & o_{24} \\ o_{31} & x_{32} & x_{33} & o_{34} \\ x_{41} & o_{42} & o_{43} & x_{44} \end{pmatrix}, \quad (1)$$

BCF can be expressed by a closed analytical formula.[13] For convenience, here we use two works  $x$  and  $o$  to denote the elements of  $\hat{\rho}_2$ , and for all the models considered in this work, it holds that  $o_{ij} = o$ . To calculate BCF, one first defines a  $3 \times 3$  matrix  $\hat{L}$  as  $L_{ij}(\hat{\rho}_2) = \text{Tr}[\hat{\rho}_2 \cdot \hat{\sigma}_i \otimes \hat{\sigma}_j]$ , with  $\{\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3\}$  the Pauli matrices. Then the BCF is given by  $B(\hat{\rho}_2) = 2\sqrt{u + v}$ , with  $u$  and  $v$  the two largest eigenvalues of the symmetric matrix  $\hat{L}^T \hat{L}$ .

In order to understand the features of nonlocality, we will compare it to two closely related measures for bipartite correlation, i.e., entanglement concurrence[27] and quantum discord[24, 25]. Concurrence describes the entanglement between two spins. Let's denote  $\tilde{\rho}_2$  as the spin-flipped matrix for the two-qubit density matrix  $\hat{\rho}_2$ , i.e.,  $\tilde{\rho}_2 = \hat{\sigma}_y \otimes \hat{\sigma}_y \hat{\rho}_2^* \hat{\sigma}_y \otimes \hat{\sigma}_y$ , then the concurrence is given by  $C = \max\{0, \mu_1 - \mu_2 - \mu_3 - \mu_4\}$ , where  $\mu_i$  are the square roots of the eigenvalues of  $\hat{\rho}_2 \tilde{\rho}_2$  in decreasing order. For separable states (in other words, unentangled states), the concurrence would vanish, and for maximum entangled states, the concurrence is 1.

Nonlocality and entanglement are two aspects of quantum correlation. Recently, quantum discord is proposed to characterize all the quantum correlation present in the system.[24, 25] Its definition is based on two quantum versions of the classical correlation. For a classical system  $AB$  composed of two subsystems  $A$  and  $B$ , the total correlation can be expressed as  $I_{A,B} = H_A + H_B - H_{AB}$ , or alternatively,  $J_{A,B} = H_A - H_{A|B}$ , with  $H_A$ ,  $H_B$  and  $H_{AB}$  the Shannon entropy, and  $H_{A|B}$  the conditional entropy.  $I_{A,B}$  and  $J_{A,B}$  are equal to each other, however, their quantum versions are found to be non-equivalent from each other, and the difference is used to define the quantum discord. By replacing the Shannon entropy and the conditional entropy with the von Neumann entropy and quantum conditional entropy, respectively,  $I_{A,B}$  becomes the quantum mutual information  $\mathcal{I}(\hat{\rho}_{AB}) = S(\hat{\rho}_A) + S(\hat{\rho}_B) - S(\hat{\rho}_{AB})$ , and the quantum extension of

$J_{A,B}$  turns out to be the classical correlation  $\mathcal{J}(\hat{\rho}_{AB}) = \max_{\{\hat{B}_k\}} \{S(\hat{\rho}_A) - S(\hat{\rho}|\{\hat{B}_k\})\}$ , where  $\{\hat{B}_k\}$  is just a complete set of projectors.[25] Finally, discord is just defined as the difference between  $\mathcal{I}(\hat{\rho}_{AB})$  and  $\mathcal{J}(\hat{\rho}_{AB})$ , i.e.,  $D(\hat{\rho}_{AB}) = \mathcal{I}(\hat{\rho}_{AB}) - \mathcal{J}(\hat{\rho}_{AB})$ . For a state containing quantum correlation, discord is generally non-zero, while for classical states,  $\mathcal{I}(\hat{\rho}_{AB})$  and  $\mathcal{J}(\hat{\rho}_{AB})$  would just reduce to  $I_{A,B}$  and  $J_{A,B}$ , respectively, thus the discord vanishes.

From the above descriptions, one can see that the entanglement concurrence and quantum discord would simply be zero in separable states and classical states, respectively.[26] As we will show in the next section, BCF can capture the signal of QPTs in these two situations.

### 3. QPTs in MPSs

In this section, we firstly give a brief introduction to MPSs, then we investigate the BCF and nonlocality at MPS-QPTs in several typical models.

An MPS containing  $N$  sites (or cells) is defined in the following matrix product form[19]

$$|\psi(g)\rangle = \sum_{i_1, \dots, i_N=1}^d \text{Tr}(\hat{A}_{i_1} \dots \hat{A}_{i_N}) |i_1, \dots, i_N\rangle, \quad (2)$$

where  $\hat{A}_i$  are  $D \times D$  matrices,  $j = 1, \dots, N$  labels the sites, and  $i_j = 1, \dots, d$  denoting the degree of freedom for site  $j$ . The matrices  $\hat{A}_i := \hat{A}_i(g)$  depend on the parameter  $g$ .

Usually, for low-dimensional quantum systems, it is difficult to express the ground-state wavefunction exactly in an explicit form. However, for an MPS  $|\psi(g)\rangle$ , one can construct a parent Hamiltonian  $\hat{H}(g)$ , which guarantees the state  $|\psi(g)\rangle$  be the ground state of  $\hat{H}(g)$ . More importantly, in the thermodynamic limit  $N \rightarrow \infty$ , as the change of  $g$ , the ground state  $|\psi(g)\rangle$  may undergo a novel type of transition, such that local observables are singular and the correlation length is divergent, with the ground-state energy keeping analytic (In traditional QPTs, the ground-state energy would be singular.)[19]. We usually say that the system undergoes an MPS-QPT.

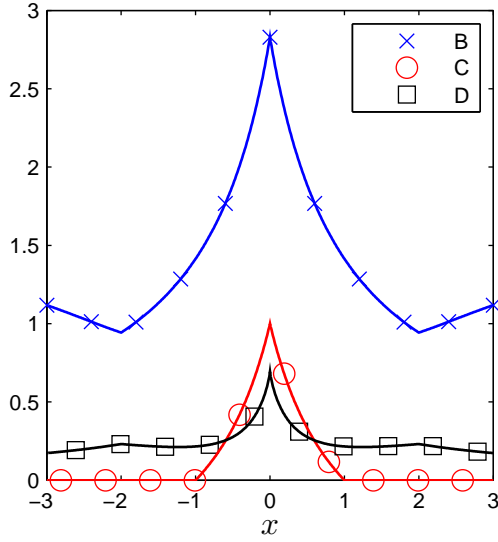
For a given MPS, the reduced density matrix of any subsystem in the system can be obtained with the help of transfer matrix technique.[20, 18, 19] First, let's define the transfer matrix  $\hat{E}$  as

$$\hat{E} = \sum_{i=1}^d \hat{A}_i^* \otimes \hat{A}_i, \quad (3)$$

then the reduced density matrix of  $k$  adjacent sites is given by

$$\rho_{i_1, \dots, i_k, j_1, \dots, j_k}(N) = \frac{\text{Tr}[(\hat{A}_{i_1}^* \dots \hat{A}_{i_k}^* \otimes \hat{A}_{j_1} \dots \hat{A}_{j_k})]}{\text{Tr}(\hat{E}^N)}. \quad (4)$$

One can further prove that, for two-site correlation, the correlation length is given by  $\xi = \frac{1}{\ln(\lambda_1/\lambda_2)}$ , where  $\lambda_1$  and  $\lambda_2$  are the first and the second largest eigenvalue of the



**Figure 1.** (Color Online) The BCF (B), concurrence (C), and discord (D) as a function of  $x = \frac{g}{2a^2}$  for the rung of the ladder. The concurrence has been investigated in Ref. [18] and is shown here just for comparison purpose.

transfer matrix  $\hat{E}$ . Any level crossing between  $\lambda_1$  and  $\lambda_2$  indicates a divergent correlation length, in other words, an MPS-QPT.[19]

In this work, we only deal with bipartite correlations. For several typical MPS models, we use Eq. (4) to obtain the reduced density matrix for the concerned two-site subsystem of the models. Then we determine the BCF, and research the behavior of BCF, concurrence and discord in the MPS-QPTs.

### 3.1. Spin ladder with four-body interaction

As the first example, we consider an MPS with  $\hat{A}_{1,2} = \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix}$ ,  $\hat{A}_3 = \begin{pmatrix} 0 & g \\ g & 0 \end{pmatrix}$ ,  $\hat{A}_4 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ . [18] Its parent Hamiltonian describes a spin  $s = \frac{1}{2}$  ladder model with SO(2) symmetry. Every rung of the ladder contains two spins with  $d = 4$ , thus four matrices are used to define the MPS. The system contains two-body bond interactions and four-body plaquette interactions.[18] As the Hamiltonian is too long, we would not show it in this work. It has been found that the ladder undergoes an MPS-QPT at  $g = 0$ , where the spin-spin correlation function of the ladder shows a singularity and the largest two eigenvalues of the transfer matrix have a level crossing.

Now we try to use quantum correlations to find the signal for the MPS-QPT. Let's just consider a single rung in the ladder. The elements of the reduced density matrix

$\hat{\rho}_2^{(\text{rung})}$  turn out to be

$$\begin{aligned} \{x_{11}, x_{44}\} &= |x| \\ \{x_{22}, x_{23}, x_{32}, x_{33}\} &= 1, \\ \{o, x_{14}, x_{41}\} &= 0 \end{aligned} \quad (5)$$

where  $x := \frac{g}{2a^2}$ . We have determined BCF on the rung and shown it in Fig. 1. The BCF shows a singularity at the MPS-QPT point  $g = 0$ , thus it can be used to detect the MPS-QPT in this model.

In addition, the first-order derivative of BCF is discontinuous at  $x = \pm 2$ . Detailed analysis shows that the singular points at  $x = \pm 2$  are due to the mathematical definition of BCF, rather than the singularity in  $\hat{\rho}_2^{(\text{rung})}$ . Explicitly, the non-physical singularity is induced by the max function in the definition of BCF. In order to calculate BCF, one has to find the two largest eigenvalues of the symmetric matrix  $\hat{L}^T \hat{L}$ . In this procedure, a mathematical singularity may emerge. In fact, a max/min function is also involved in the definition of the discord/concurrence. As a result, the concurrence and discord can also show a non-physical singularity, just as shown in Fig. 1.

Now let's discuss the feature of quantum correlation in the rung. As indicated by the discord in Fig. 1, quantum correlation exists for any finite  $x$ . In the vicinity of the MPS-QPT point, that is, for  $|x| < 0.41$ , it's found that the concurrence is non-zero and  $B > 2$ , thus the quantum correlation is in the form of both entanglement and nonlocality. While for  $0.41 < |x| < 1$ , the concurrence is non-zero and  $B < 2$ , thus the quantum correlation is in the form of entanglement without nonlocality. For  $|x| > 1$ , it is present neither in the form of entanglement nor in the form of nonlocality. It shows clearly that quantum correlation can be manifested by various forms.

### 3.2. XYZ interaction model

Let's consider an MPS with  $\hat{A}_1 = \begin{pmatrix} 1 & g \\ 1 & 1 \end{pmatrix}$  and  $\hat{A}_2 = \begin{pmatrix} 1 & -g \\ -1 & 1 \end{pmatrix}$ . After the standard procedure, one can construct its parent Hamiltonian as [20]

$$\hat{H} = \sum_{i=1}^N J_x \hat{\sigma}_x^i \hat{\sigma}_x^{i+1} + J_y \hat{\sigma}_y^i \hat{\sigma}_y^{i+1} + J_z \hat{\sigma}_z^i \hat{\sigma}_z^{i+1} - B \hat{\sigma}_z^x, \quad (6)$$

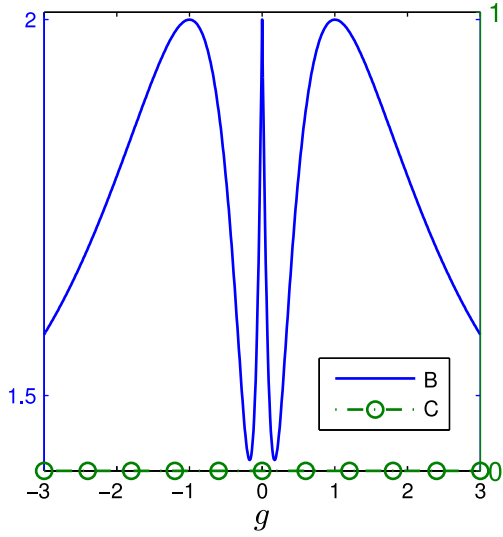
with  $J_x = -J + \frac{1}{2}(1 + g^2)$ ,  $J_y = -J + g$ ,  $J_z = -J - g$  and  $B = 1 - g^2$ . It is just an XYZ interaction chain. It has been proved that the system has an MPS-QPT at  $g = 0$ . [20]

Firstly, we consider the correlation between two nearest-neighboring spins  $i$  and  $i + 1$ . For  $g > 0$ , the corresponding reduced density matrix  $\hat{\rho}_2^{(i, i+1)}$  is given by

$$\begin{aligned} \{x_{11}, x_{44}\} &= g^2 + 6g + 1 \\ \{x_{22}, x_{23}, x_{32}, x_{33}, x_{14}, x_{41}\} &= (g - 1)^2, \\ o &= 1 - g^2 \end{aligned} \quad (7)$$

while for  $g > 0$ , one finds that

$$\begin{aligned} \{x_{14}, x_{41}\} &= g^2 + 6g + 1 \\ \{x_{22}, x_{23}, x_{32}, x_{33}, x_{11}, x_{44}\} &= (g - 1)^2. \\ o &= 1 - g^2 \end{aligned} \quad (8)$$



**Figure 2.** (Color Online) The BCF (B) as a function of  $g$  for any two spins in the XYZ interaction model. The concurrence (C) has been investigated in Ref. [20] and is shown here just for comparison purpose.

Previous studies show that  $\hat{\rho}_2^{(i,i+1)}$  is separable for any  $g$ , thus the bipartite entanglement between  $i$  and  $i + 1$  vanishes and cannot detect the MPS-QPT of the system.[20, 23] From Fig. 2 we find that BCF is generally non-zero in the whole parameter space and shows a singularity at the MPS-QPT point  $g = 0$ .

In fact, for any two-site subsystems of the model, the reduced density matrix  $\hat{\rho}_2^{(i,i+r)}$  does not depend on the distance  $r$  at all.[20] As a result, the concurrence for any two-site subsystem is zero, thus bipartite entanglement cannot detect the QPT of the system while the BCF can do the job very well. This example shows clearly that BCF can detect QPTs in separable states while entanglement fails.

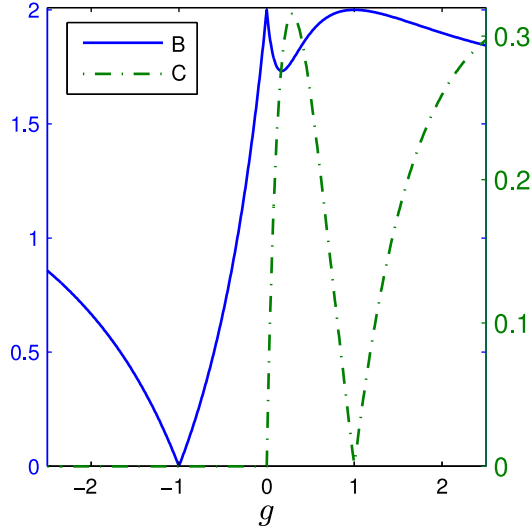
We observe that the Bell-CHSH inequality is not violated in the MPS-QPT in this XYZ interaction model. We'd like to mention that the quantum correlation indeed exists in the QPT region, indicated by the discord.[23] It is interesting that the quantum correlation present in  $\hat{\rho}_2^{(i,i+r)}$  is neither in the form of entanglement nor in the form of nonlocality.

### 3.3. Three-body interaction model

We consider an MPS with  $\hat{A}_1 = \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}$  and  $\hat{A}_2 = \begin{pmatrix} 1 & g \\ 0 & 0 \end{pmatrix}$ . Its parent Hamiltonian describes a three-body interaction model as follows [19]

$$\hat{H} = \sum_{i=1}^N J_3 \hat{\sigma}_z^i \hat{\sigma}_x^{i+1} \hat{\sigma}_z^{i+2} + J_z \hat{\sigma}_z^i \hat{\sigma}_z^{i+1} - B \hat{\sigma}_i^x, \quad (9)$$

with  $J_3 = (g - 1)^2$ ,  $J_z = 2(g^2 - 1)$ , and  $B = (1 + g)^2$ . The system undergoes an MPS-QPT at  $g = 0$ . [19]



**Figure 3.** (Color Online) The BCF (B) as a function of  $g$  for nearest-neighboring two sites in the three-body interaction model. The concurrence (C) has been investigated in Ref. [23] and is shown just for comparison purpose.

We consider the two-qubit states  $\hat{\rho}_2^{(i,i+r)}$  in the chain with different  $r$ . When  $r = 1$ , the reduced density matrix for  $g > 0$  is given by

$$\begin{aligned} \{x_{11}, x_{44}\} &= \frac{g+1}{2}, \quad \{x_{22}, x_{33}\} = \frac{g^2+g}{2} \\ \{x_{23}, x_{32}\} &= \frac{2g^2}{g+1}, \quad \{x_{14}, x_{41}\} = \frac{2g}{g+1}, \\ o &= g \end{aligned} \quad (10)$$

while for  $g < 0$ ,  $\hat{\rho}_2^{(i,i+1)}$  is a diagonal matrix, with the diagonal entries given by

$$\{x_{11}, x_{44}\} = 1, \quad \{x_{22}, x_{33}\} = -g, \quad (11)$$

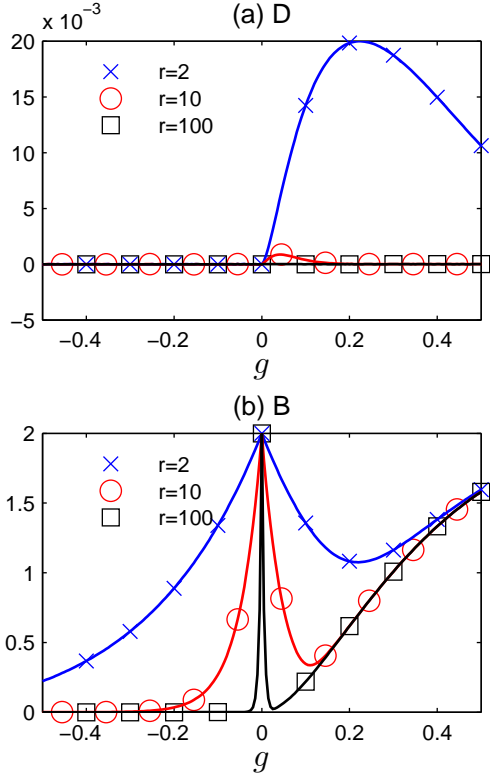
which denotes a classical state. The BCF is shown in Fig. 3. BCF shows a singularity at  $g = 0$ , thus it can be used to detect the MPS-QPT of the model. In addition, BCF is singular at  $g = -1$ . Detailed analysis shows that this singular point results from the mathematical definition of BCF, rather than a transition in  $|\psi(g)\rangle$ . For  $g > 0$ , we observe that  $\hat{\rho}_2^{(i,i+1)}$  never violate the Bell inequality, despite being entangled. In other words, the quantum correlation in nearest-neighboring sites is in the form of entanglement, rather than nonlocality.

Next, we consider two sites  $i$  and  $i + r$  with  $r \geq 2$ . For  $g > 0$ , the elements of the reduced density matrix  $\hat{\rho}_2^{(i,i+r)}$  are given by

$$\begin{aligned} \{x_{11}, x_{44}\} &= 1 + \left(\frac{1-g}{1+g}\right)^r \\ \{x_{22}, x_{33}\} &= 1 - \left(\frac{1-g}{1+g}\right)^r \\ \{x_{14}, x_{23}, x_{32}, x_{41}\} &= \frac{16g^2}{(1+g)^4}, \\ o &= \frac{4g}{(1+g)^2} \end{aligned} \quad (12)$$

while for  $g < 0$ ,  $\hat{\rho}_2^{(i,i+r)}$  is reduced to a diagonal matrix, with the diagonal elements given by

$$\{x_{11}, x_{44}\} = 1 + \left(\frac{1+g}{1-g}\right)^r, \quad \{x_{22}, x_{33}\} = 1 - \left(\frac{1+g}{1-g}\right)^r. \quad (13)$$



**Figure 4.** (Color Online) The quantum discord (D) and the BCF (B) as a function of  $g$  for two sites  $i$  and  $i+r$  in the three-body interaction model.

We numerically found that the concurrence vanishes in the whole parameter space for  $r \geq 2$ , which means that  $\hat{\rho}_2^{(i,i+r)}$  is separable. Previous study shows that quantum discord may be able to capture the signal of QPT in separable states[26, 23]. We have calculated the discord for different  $r$  and the result is shown in Fig. 4(a). One can see that the value of discord is very small even for  $r = 2$ . As the increase of the distance  $r$ , the discord decreases rapidly. Finally, for a large  $r$ , the two-qubit state  $\hat{\rho}_2^{(i,i+r)}$  would become a classical state without any quantum correlation, thus neither the concurrence nor the discord can signal the MPS-QPT of the system. Then let's study the BCF for  $\hat{\rho}_2^{(i,i+r)}$ . From Fig. 4(b) one sees clearly that BCF shows a singularity at the QPT point  $g = 0$  for any finite  $r$ . Thus, BCF is able to capture the singularity in classical states, for which both the concurrence and the discord fail. In addition, our results show that the Bell-CHSH inequality is never violated, thus the quantum correlation between the non-nearest-neighbor spins, if exists, is neither in the form of entanglement, nor in the form of nonlocality.

#### 4. Summaries and discussions

In this work, for several typical models, we find that BCF can be used to detect the MPS-QPTs very well. The underlying mechanism is as follows. Our discussion applies

to MPS-QPTs and traditional QPTs. When a QPT occur, some local observables, such as spin-spin correlation functions, would be singular at the QPT point.[28] These correlation functions can be used to construct the reduced density matrix  $\hat{\rho}_2(g)$ .[29] As a result, the QPT and the singularity in  $\hat{\rho}_2(g)$  are closely related to each other. The BCF, concurrence and discord, defined based upon  $\hat{\rho}_2(g)$ , may capture the singularity in  $\hat{\rho}_2(g)$ , thus, all the three quantities can be used to detect the QPTs.

In Ref. [5] a general argument for why BCF should be as good as entanglement to signal QPTs has already been made. Now let's discuss the advantage of BCF in detecting QPTs. BCF can capture singularity in unentangled states and classical states, for which entanglement and discord fails, respectively. Quantum discord is defined on the classical-quantum paradigm from a measurement perspective, thus it captures all the quantumness of correlation in the system. For classical states, discord is zero thus loses its function as a QPT indicator. This is just the situation for  $\hat{\rho}_2^{(i,i+r)}$  with  $r > 1$  in the three-body interaction model. On the other hand, quantum entanglement is defined on the separability-entanglement paradigm. For quantum separable states, it is zero thus would lose the signal of QPT in these states. This is just what happens in any two-site subsystem in the XYZ model. BCF is used to detect the nonlocality of a state. For non-local states, it would be larger than 2, while for most local states, it does not vanish. In extreme cases, even if the state is a classical state thus  $\hat{\rho}_2$  is diagonal, the BCF would turn out to be  $B = 2|x_{11} + x_{44} - x_{22} - x_{33}|$ , which is still non-zero unless  $x_{11} + x_{44} = x_{22} + x_{33}$ . As a result, BCF can detect the singularity in various density matrices, including separable/entangled states, local/non-local states, and classical/quantum states.

Now we clarify the drawback of BCF. First of all, for a general state, the calculation of BCF is difficult, which greatly limits its application. In addition, as shown in  $x = \pm 2$  of Fig. 1 and  $g = -1$  of Fig. 3, the mathematical definition of BCF can introduce non-physical singularity, which is not related to the singularity in  $\hat{\rho}(g)$ . As a result, the singularity of BCF just can be used to detect, rather than to determine, an MPS-QPT. However, we'd like to mention that both the concurrence and the discord have similar disadvantage (see Fig. 1 as examples), which has already been discussed in some other studies.[26, 8]

Let's discuss the form of quantum correlation in the MPS-QPTs of these models. In this work, we have only dealt with bipartite correlations. We use the discord to identify the existence of quantum correlation, and then describe the nature of quantum correlation through the analysis of entanglement and nonlocality. In the vicinity of MPS-QPT point in the ladder model, the quantum correlation in  $\hat{\rho}_2^{(\text{rung})}$  is in the form of both entanglement and nonlocality. In the three-body interaction model, for  $\hat{\rho}_2^{(i,i+1)}$ , the quantum correlation is in the form of entanglement without nonlocality, while for  $\hat{\rho}_2^{(i,i+r)}$  with  $r > 1$ , the quantum correlation, if exist, is neither in the form of entanglement nor nonlocality. In the XYZ interaction model, for any two spins in the chain, the quantum correlation is neither in the form of entanglement nor nonlocality. From one hand, our results show that when MPS-QPTs occur, the two-site quantum

correlation can show very rich nature combined with entanglement and nonlocality. From another hand, it reveals that entanglement and nonlocality are not the only aspects of quantum correlation, and there exists some kind of quantum correlation which cannot be characterized by entanglement, nor by nonlocality.

Finally, as we have shown in this work, the Bell-CHSH inequality is violated just in the QPT of the four-body interaction ladder model. In fact, as far as we know, in all the previous works, [16, 5, 6] when QPTs occur in infinite models, the density matrices of two-qubit subsystems never violate the Bell-CHSH inequality. Thus, the ladder model reported in this work may be the first one to present such a behavior. In QPTs in many-body systems, as an important aspect of quantum correlation, nonlocality should play a central role, however, it turns out that bipartite nonlocality is not a common form of quantum correlation present in these one-dimensional systems.

We'd like to mention that, for many-body systems, which are naturally multipartite, it would be more natural for quantum correlation to present in the form of multipartite nonlocality.[35, 30, 31] It has been found that Bell inequalities can be used to test multipartite nonlocality.[32] In addition, effective approaches to detect or even quantify multipartite nonlocality have been proposed.[33, 34]

However, the relevance of multipartite nonlocality in QPTs remains unknown. As bipartite nonlocality is not favored at the QPT points in many one-dimensional models, it would be interesting to clarify whether multipartite nonlocality is significant in QPTs. Considering the simple product form of MPSs, we believe MPS models would be very useful to study this important issue.

After finishing this manuscript, we become aware of a related work [36] by Oliveira et. al. The authors have proposed a general explanation for why the Bell inequality is not violated in most translation invariant systems. Then they have shown that the inequality can be violated for models with translation symmetry breaking. Our results of the spin ladder model suggest that, for two spins located in a unit-cell of a complex lattice, the Bell inequality can still be violated in a translation invariant system.

## Acknowledgment

The research was supported by the National Natural Science Foundation of China (No. 11204223). This work was also supported by the Talent Scientific Research Foundation of WHPU (No. 2012RZ09 and 2011RZ15), and China Postdoctoral Science Foundation (No. 2012M510342).

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